MGI at ONR

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Director, Naval Materials Division
January 11, 2016

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The Office of Naval Research

The S&T Provider for the Navy *and* Marine Corps

- 4,000+ People
- 23 Locations
- $2.1B / year
- >1,000 Partners

Discover → ***Develop*** → ***Deliver*** → ***Technological Advantage***

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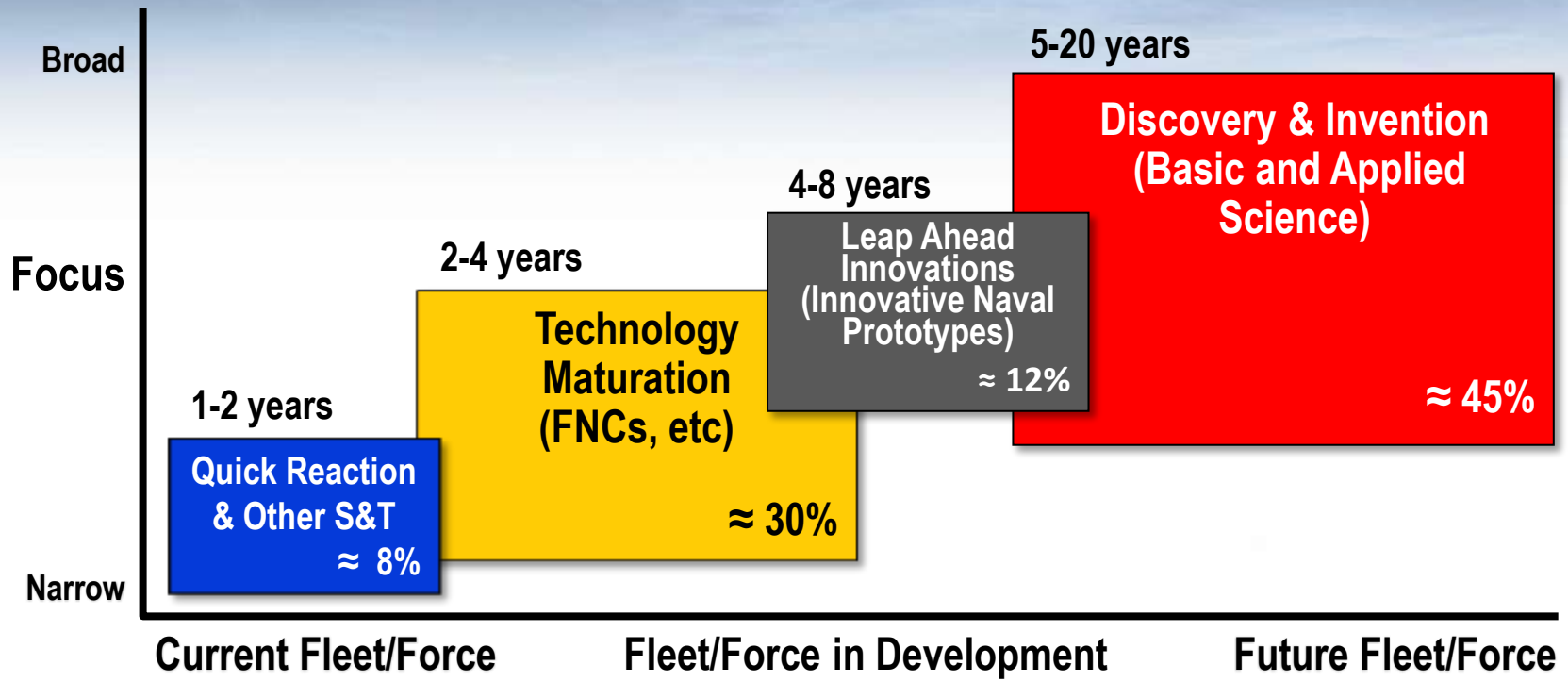
Warfighting Capabilities Enabled by S&T Investments



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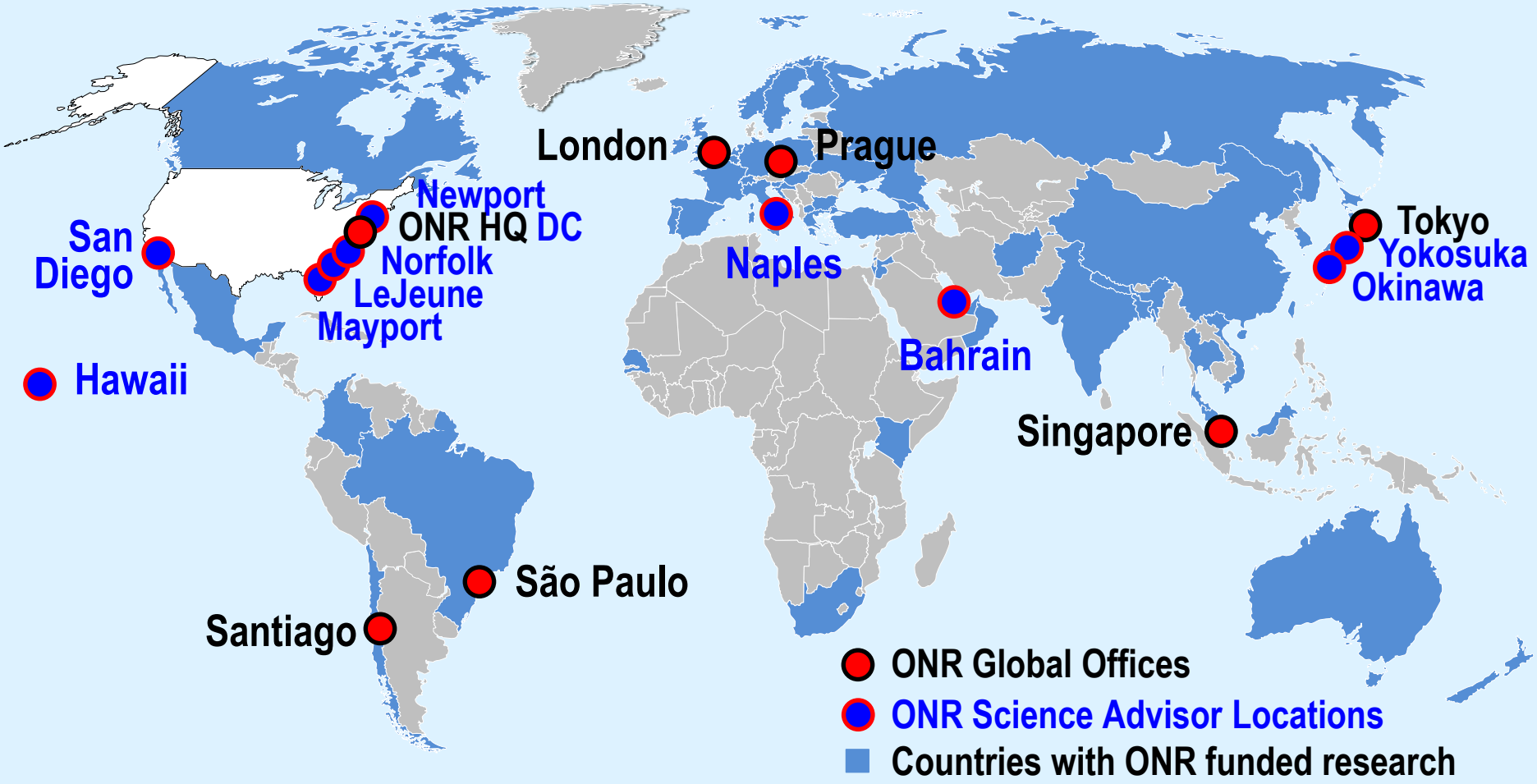
Global & Fleet Engagement



We execute $2B/year with the Naval S&T community in the US and 55 countries

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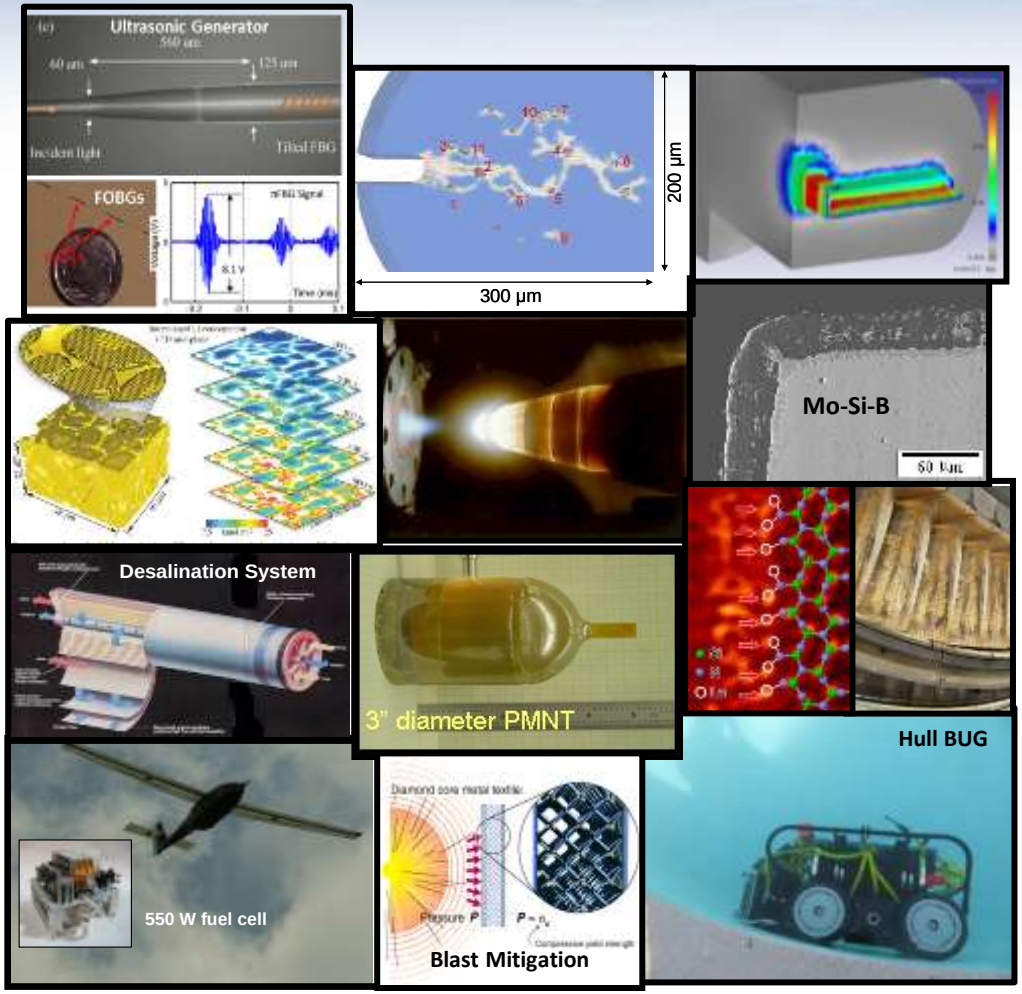
Naval Materials S&T

Integrated theoretical, computational and experimental programs to understand and develop the physics, chemistry, materials and processing that confidently meet critical naval needs



High Performance Functional Materials

- Power Generation & Energy Storage Materials
  - Electrochemical Materials
  - Polymeric and Organic Materials
- Piezoelectric Materials

High Performance Structural Materials

- Structural Metallic, Structural Cellular and Composite Materials
- High Temperature Turbine and Ultra-high Temperature Materials
- Welding and Joining
- Optical Ceramics

Environmental Quality

- Anti-fouling Release Coatings
- Solid and Liquid Waste Treatment

Optimization from Design thru System Life

- Computer Aided Materials Design
- Scarce Element Mitigation Strategies
- Solid Mechanics and Fatigue
- Non-Destructive Evaluation and Prognostics
- Integrated Computational Materials Engineering

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Naval Interests

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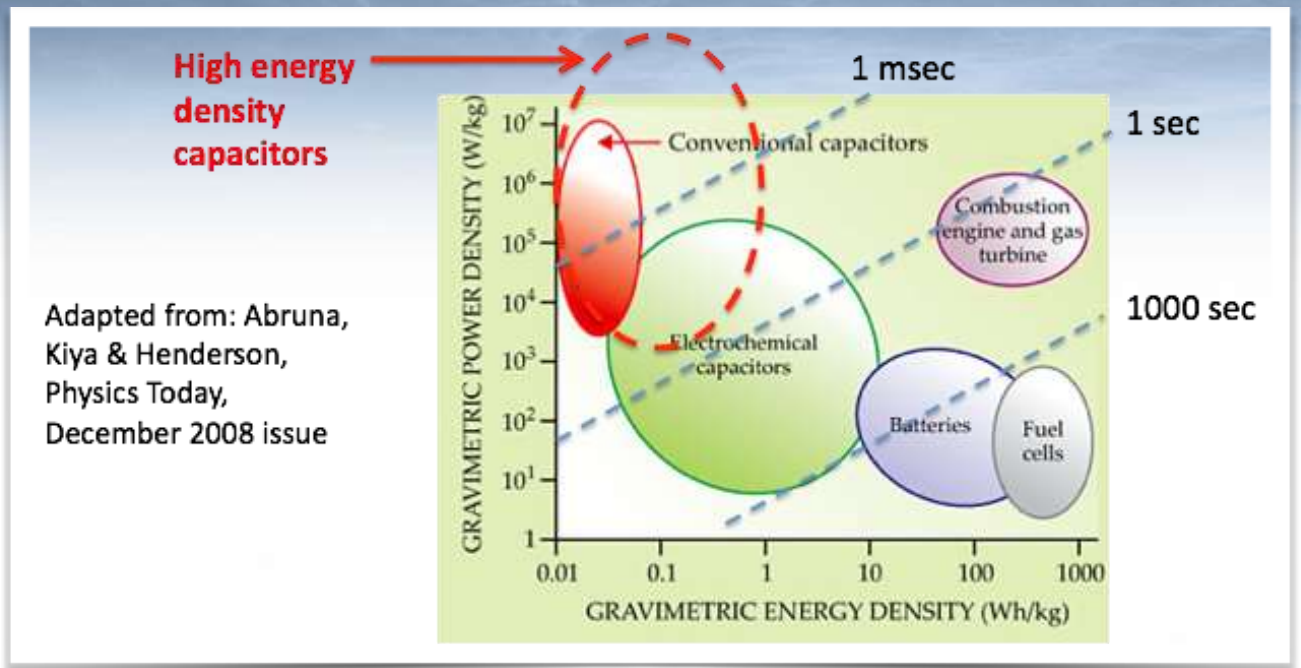
Energy Storage Challenges



Capacitors are the only option for rapid discharge (e.g., pulsed power) applications

State of the Art: Biaxially-oriented polypropylene (BOPP)

- High breakdown field (700 V/μm); Low loss (0.0001); Cheap
- But, low dielectric constant of 2.2 ⟶ Energy density of 5 J/cc

Maximum Energy Density = (dielectric constant)(breakdown field)^2

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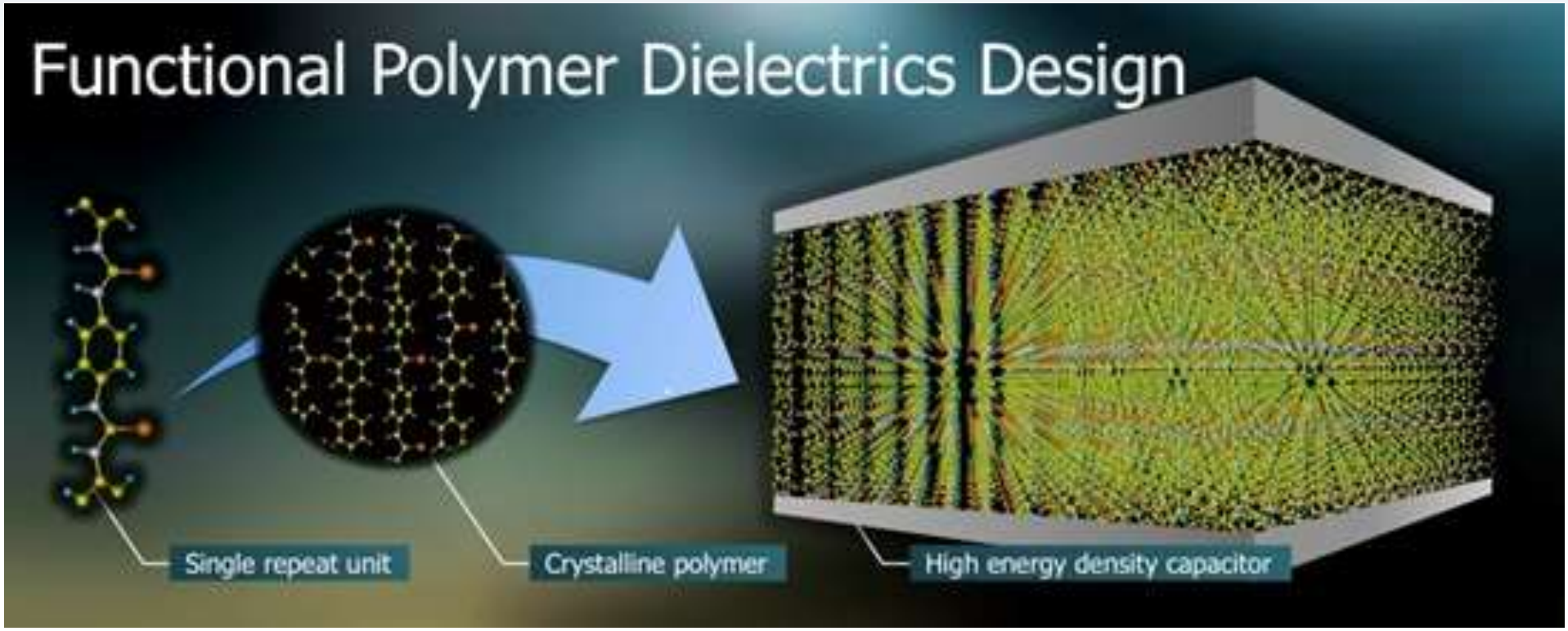
Rational Design of Polymer Dielectrics via
Synergistic Computations, Synthesis & Characterization



Rampi Ramprasad, U. Connecticut
MURI Team Leader

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Rational Design of Polymer Dielectrics via
Synergistic Computations, Synthesis & Characterization

Bob Weiss
Synthesis
characterization

Rampi Ramprasad
Ab initio modeling & Data mining

Yang Cao, Steve Boggs
Electrical characterization

Miko Cakmak
Processing

Sanat Kumar
Classical modeling

Greg Sotzing
Synthesis

Mike Chung
Synthesis

Curt Breneman
Informatics modeling

The University of Akron | Columbia University in the City of New York | University of Connecticut | PennState | Rensselaer

Rational Design of Advanced Polymeric Capacitor Films

www.ims.uconn.edu/MURI

Multidisciplinary University Research Initiative (MURI)

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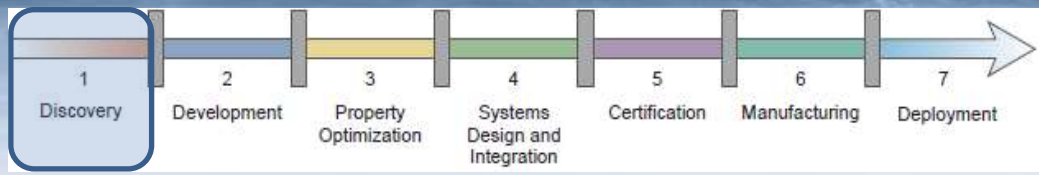
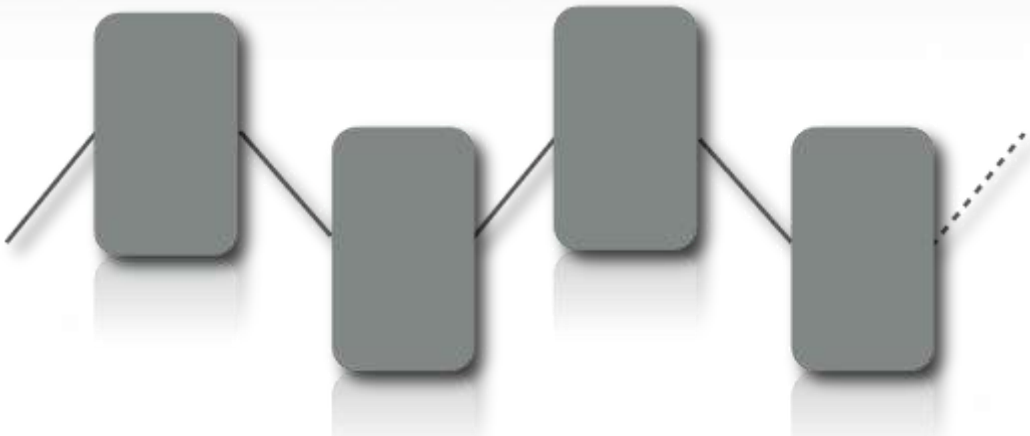
High Throughput Screening





Organic Blocks: CH_2, CO, CS, O, NH, C_6H_4, C_4H_2S

"Rational Design of All-Organic Polymer Dielectrics", Sharma, et al, Nature Communications (2014)

Hybrid Blocks: CH_2, SiF_2, $SiCl_2$, GeF_2, $GeCl_2$, SnF_2, $SnCl_2$, O, $Sn(CH_3)_2$

"Poly(dimethyltin glutarate) as a Prospective Material for High Dielectric Applications", Baldwin, et al, Advanced Materials (2015)

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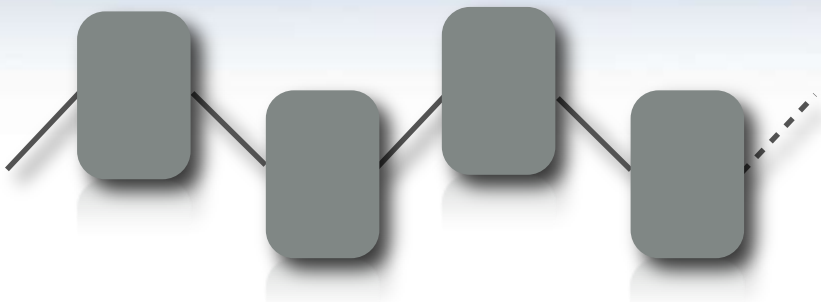
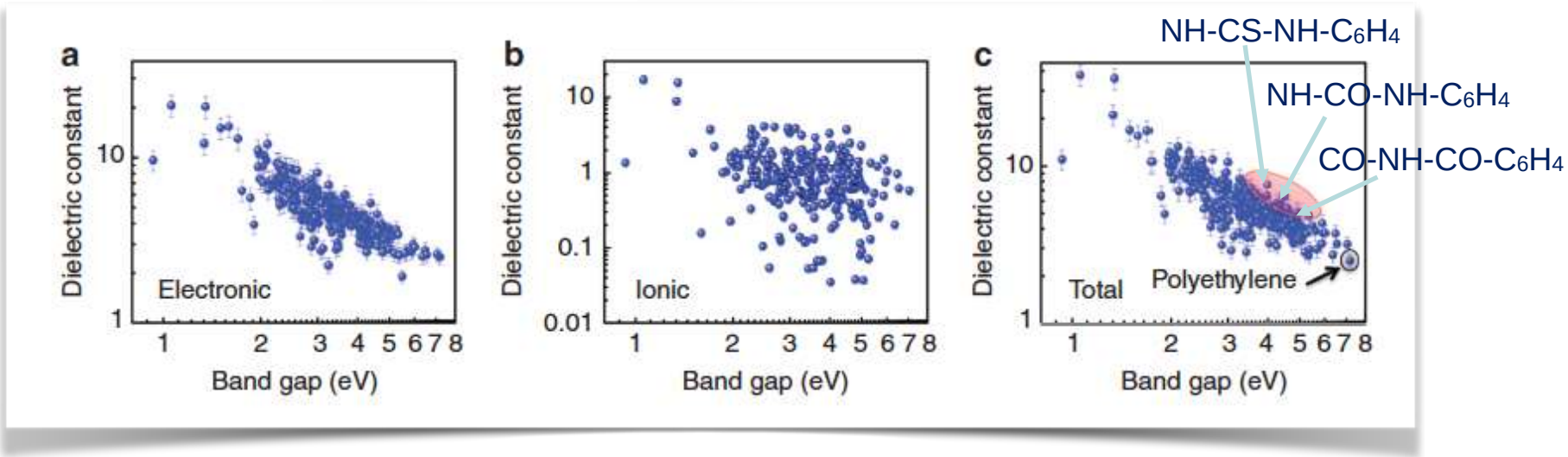
High Throughput Screening

Blocks ∈ {CH_2, CO, CS, O, NH, C_6H_4, C_4H_2S}



~ 300 Systems in Total



High-throughput DFT leads to promising polymers

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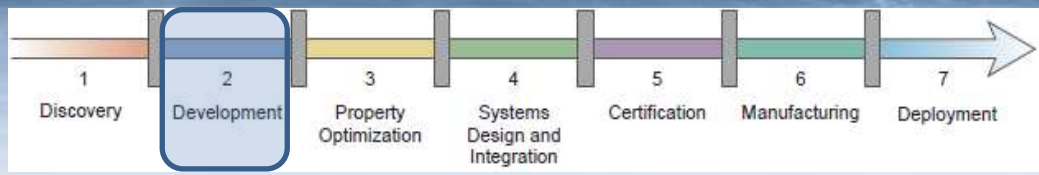
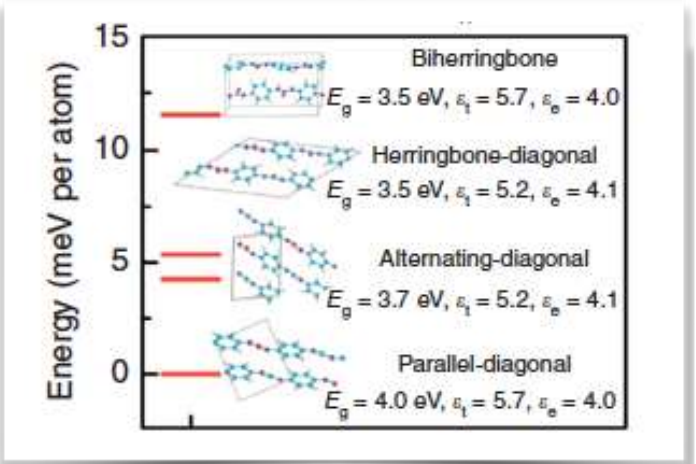
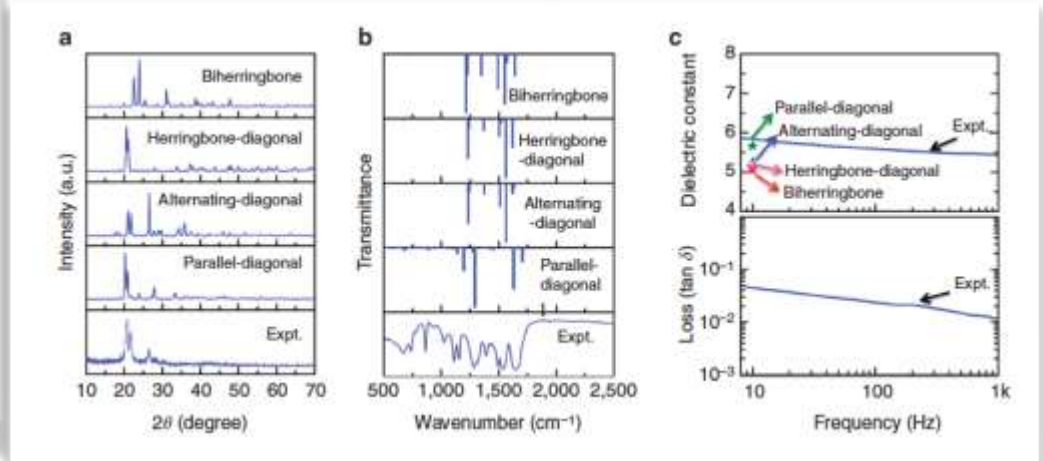
3D Structure & Properties



Computations versus measurements for NH-CO-NH-C_6H_4 (polyurea)





- Constrained evolutionary search (based on DFT energies)
- Melt-and-quench based search (based on OPLS force field)

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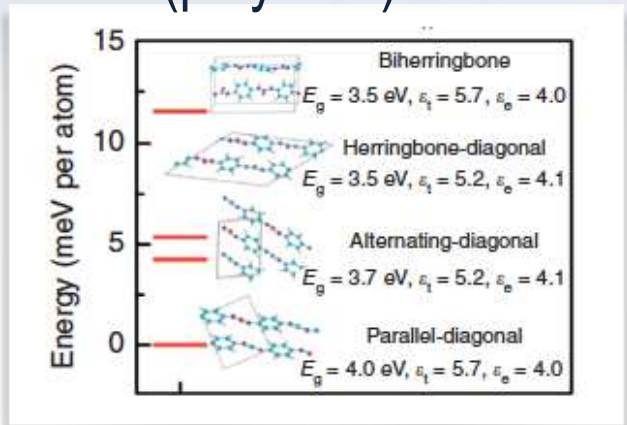
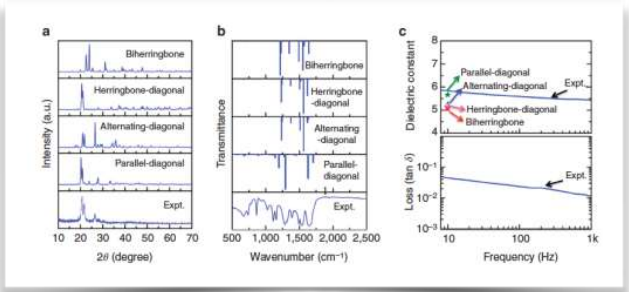
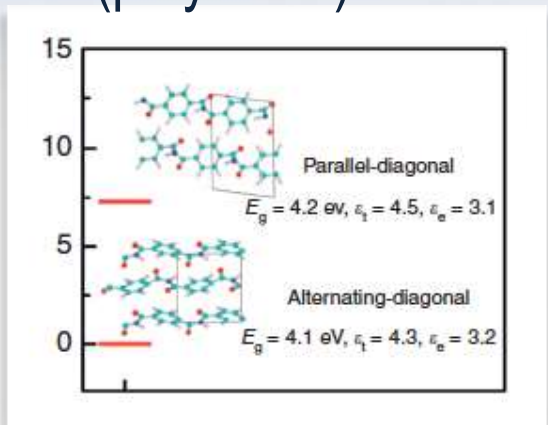
3D Structure & Properties

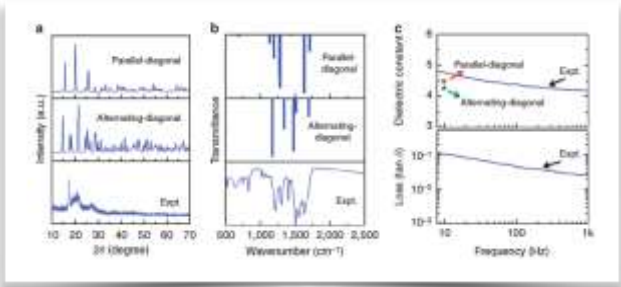
NH-CO-NH-C_6H_4 (polyurea)



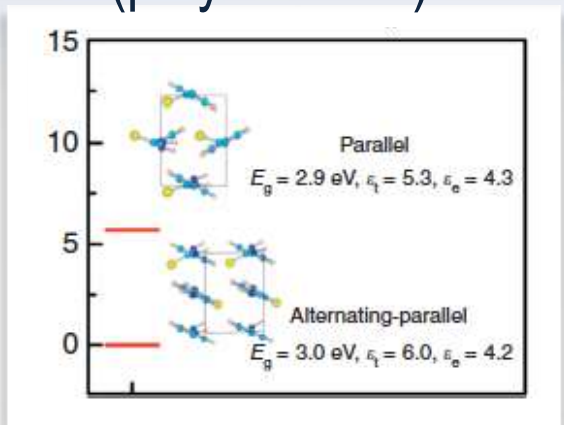


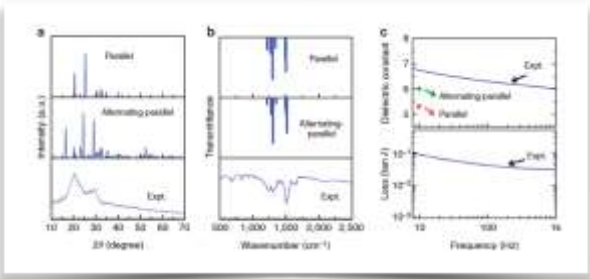
CO-NH-CO-C_6H_4 (polyimide)





NH-CS-NH-C_6H_4 (polythiourea)





But none of them is "processable", i.e., flexible thin films cannot be made!

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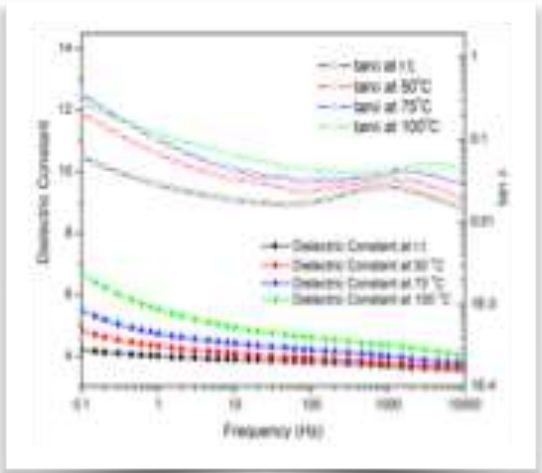
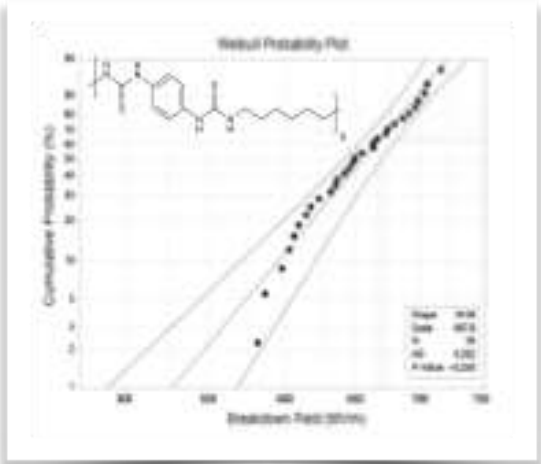
1st Co-Design Product

Breakdown field competitive with BOPP (current standard), with dielectric constant twice the value.

$[NH\text{-}CS\text{-}NH\text{-}C_6H_4\text{-}NH\text{-}CS\text{-}NH\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}CH_2\text{-}]_n$





Ma, et al, “Rational design and synthesis of polythioureas as capacitor dielectrics”, J. Mater. Chem. A 3, 14845 (2015)
[See also Shan Wu, et al, J. Electronic Materials (2014)]

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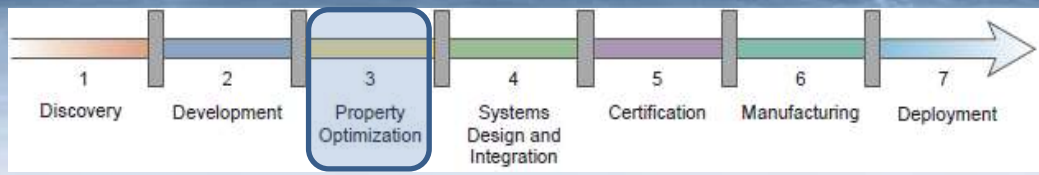
Further Exploration

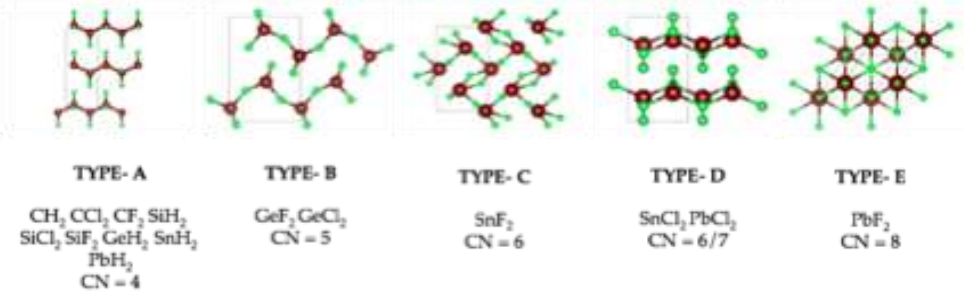


... by ushering in Group 14 elements?

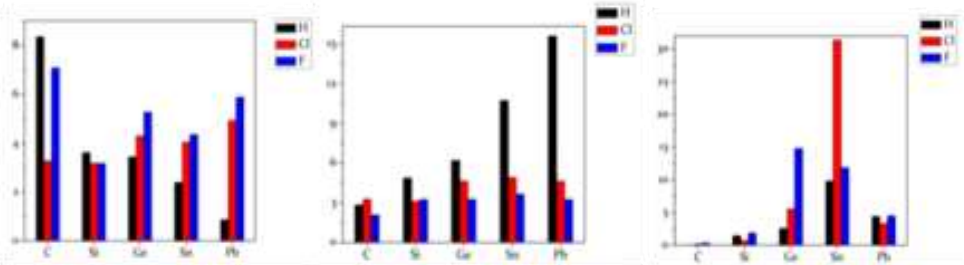
Wang, et al, Phys. Rev. B 87, 035103 (2013);

Mannodi-Kanakkithodi, et al, J. Mater. Sci. (2014)

Coordination chemistry across Group 14 hydrides and halides!



Property variation across Group 14 hydrides and halides!



HSE Band Gaps (eV) | Electronic Dielectric Constant | Ionic Dielectric Constant

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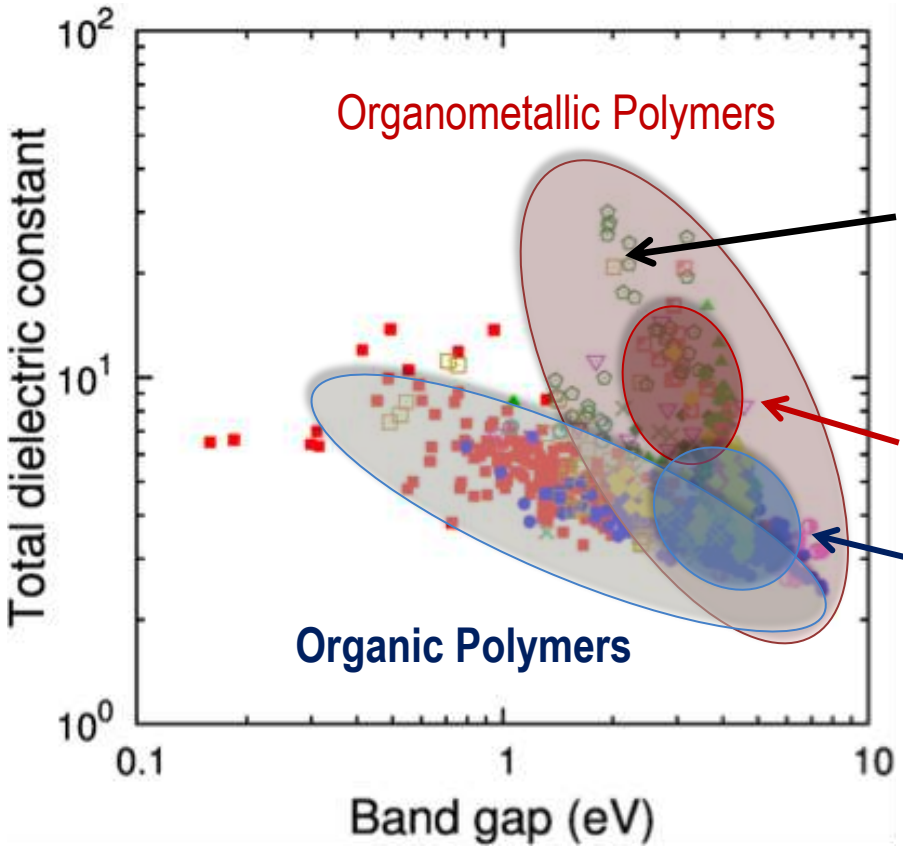
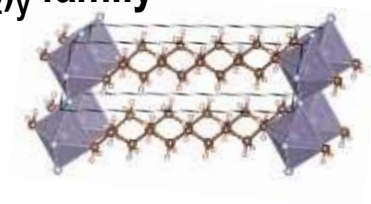
2nd Co-Design Product



$-(SnF_2)_x-(CH_2)_y$ family



Sn esters

ureas, imides, etc.

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Khazana (University of Connecticut)

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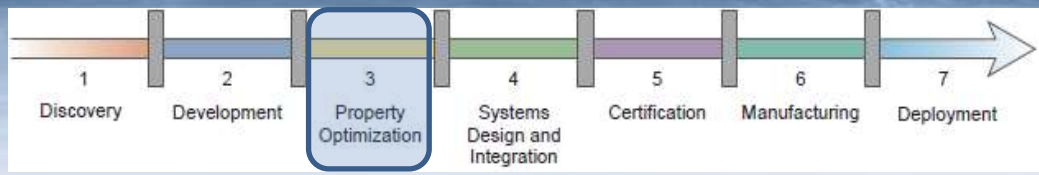
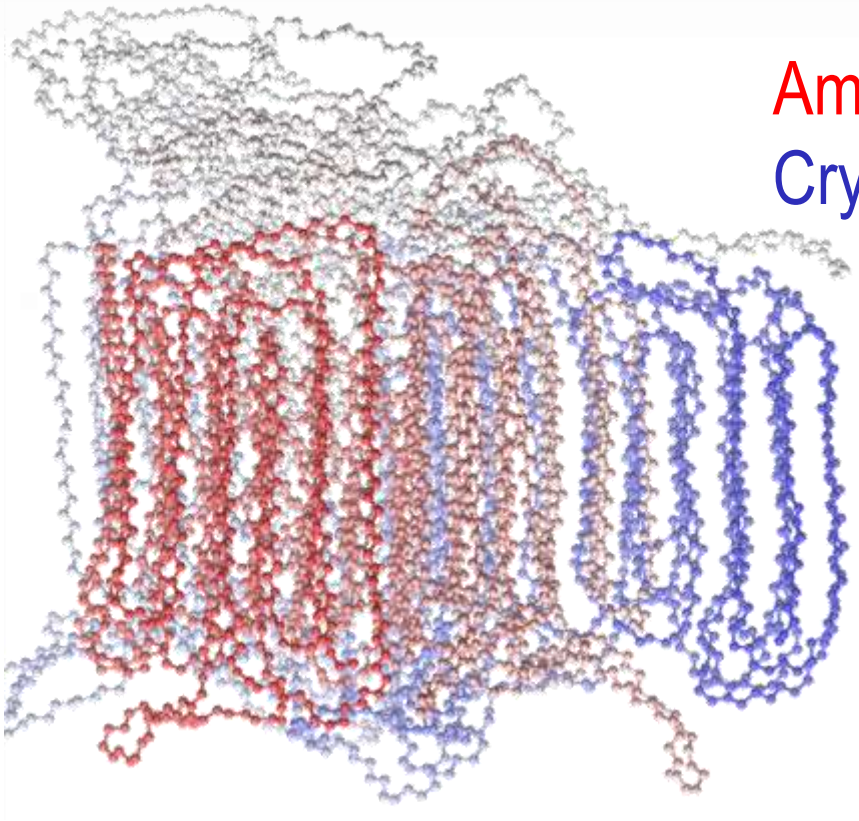
Understanding and Controlling Morphology





Amorphous

Crystalline

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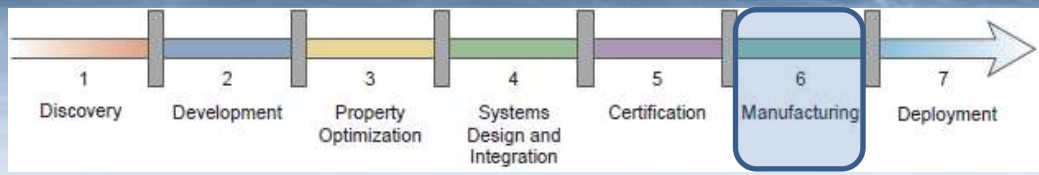
Dielectric Film Processing



Polymers like polypropylene (PP), polyamide (PA), etc. are extruded, cast, and mechanically stretched under the influence of heat.

Stretching modifies the molecular structure and thickness of the film, yielding specific properties.

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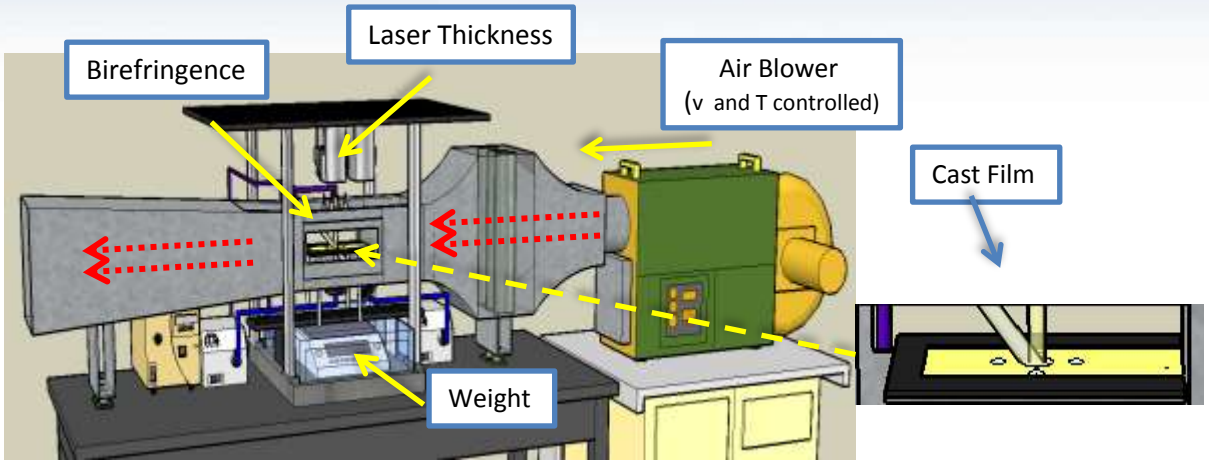
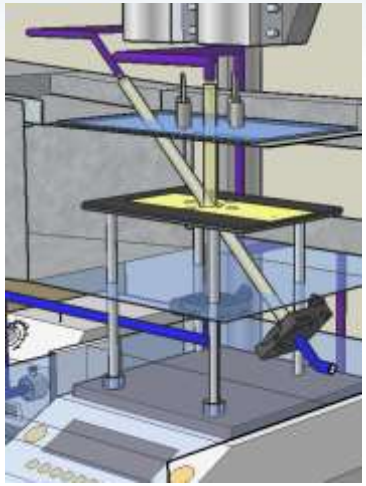
Processing for Structure

Real-time monitoring of drying behavior and polymer chain orientation





Real-time measurements

- Thickness
- Weight
- Surface temperature
- In-plane, out-of-plane birefringence
- Video capture

→

Information

- Real-time development of local chain orientation in films as they are being dried
- Suitable conditions for solvent-casting (casting temperature, polymer conc. etc.)
- Time required to reach steady-state

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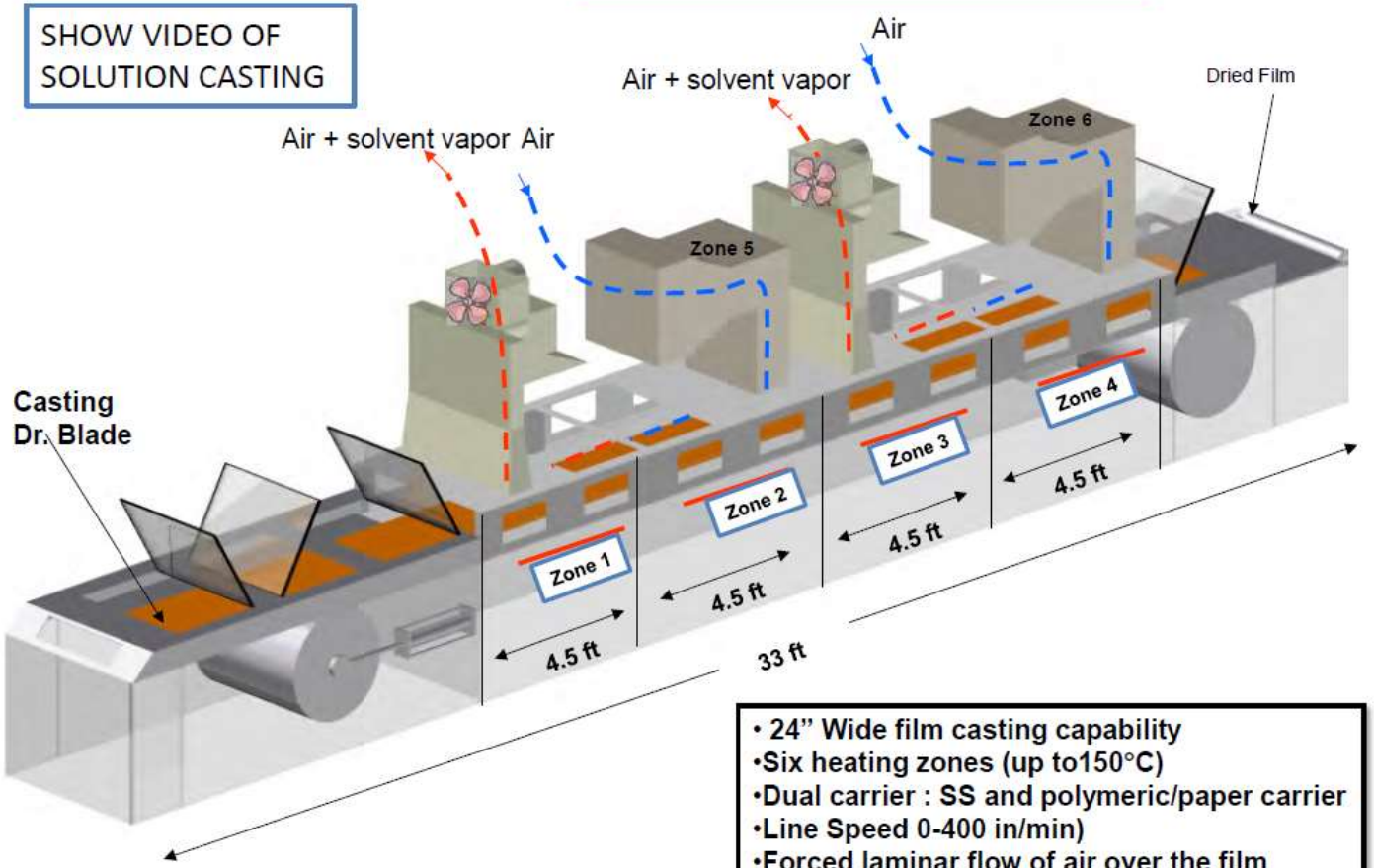
Informed Manufacturing Schemes

SOLUTION PROCESSING

SHOW VIDEO OF SOLUTION CASTING

CASTING OF POLYIMIDE PRECURSORS



- 24" Wide film casting capability
- Six heating zones (up to150°C)
- Dual carrier : SS and polymeric/paper carrier
- Line Speed 0-400 in/min)
- Forced laminar flow of air over the film

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Innovative Manufacturing Institutes

Advanced Manufacturing Partnership-

Active and Planned Institutes

- National Additive Manufacturing Innovation Institute (NAMII)
  - a.k.a. America Makes (DoD/DOE) FY12
- Digital Manufacturing and Design Innovation Institute (DMDII)
  - (DoD) FY14
- Lightweight and Modern Metals Manufacturing Innovation Institute
  - a.k.a. LIFT(DoD) FY14
- Next Generation Power Electronics Manufacturing Innovation Institute
  - a.k.a. Power America (DOE) FY14
- Clean Energy Manufacturing Innovation Institute for Composites Materials and Structures
  - a.k.a. IACMI (DOE) FY15
- American Institute for Manufacturing Integrated Photonics
  - a.k.a. AIM Photonics (DoD) FY15
- Flexible Hybrid Electronics Manufacturing Institute
  - a.k.a NEXTFLEX (DoD) FY15

http://manufacturing.gov

Lightweight Innovations for Tomorrow (lift)

Lightweight & Modern Metals Manufacturing Innovation Institute (LM3II)

Build a Systems Engineering Approach to Advanced Manufacturing

Objectives

- Metal Foci: Al, Mg, Ti, other modern metals
- Four themes
  - Production Scale-up (MRL 4-7)
  - Shorten Design-to-Production Cycle
  - Affordable Manufacturing Processes
  - Tools, Skills, Knowledge for Manufacturing Workforce, from Design to Manufacturing
- **Integrated design, metals processing, and manufacturing of PRODUCTS**

Application Areas

- Application of new/novel metals and alloys
- Primary metal manufacturing
- Secondary metal manufacturing
- Development of products exploiting lightweight and modern metals

Approach:

- Establish partnerships with industry program managers and manufacturing technology developers
- Require early identification of key performance parameters (KPPs) and co-development of component and manufacturing processes enabled by ICME
- Engage community colleges and industrial training programs to ensure an able workforce

Warfighter Benefits/Impacts

- Improved maneuverability, transportability, speed, and range of military vessels, vehicles, and systems
- Increased payload capacity (weight) in the form of weapons, equipment, personnel, or materiel loads
- Reduced fuel consumption and costs, including support requirements
- Enhanced affordability

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